DSMC Study of Shock-Detachment Process in Hypersonic Chemically Reacting Flow

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Abstract. Hypersonic chemically reacting flow around a wedge in the near-continuum regime was numerically studied by the DSMC method with the main goal of validation of real gas effect models. The influence of vibration-dissociation coupling on the results of numerical simulations was analyzed. To this end, two models of chemical reactions were used in the computations, the total collisional energy model and a vibrationally favored model. The numerical results were compared with the experimental data of Hornung and Smith on the shock-wave stand-off distance in a hypersonic flow around the wedge. Sensitivity of simulation results to chemical reaction rate constants was also estimated.

INTRODUCTION

The Direct Simulation Monte Carlo (DSMC) method is currently one of the main tools for modeling gas flows around re-entry vehicles at high altitudes. An important aspect of the method is the development and validation of models that describe real gas effects: translational-internal nonequilibrium and chemical reactions, which significantly affect the flow structure around the vehicle and heat loads on its surface. Validation of DSMC models of real gas effects is a complicated problem because the experimental data on high-enthalpy gas flows are available mostly for the continuum flow regime (Knudsen numbers Kn less than 10^{-5}). 2D and 3D DSMC simulations of such flows are beyond the capabilities of existing computers. An example of the scarce data suitable for validation of real gas effect models for the DSMC method is the experimental results presented in [1]. Principal attention was paid in these experiments to the effects of thermal relaxation and dissociation on the shock-wave stand-off distance for a flow about a wedge placed symmetrically in a uniform hypersonic flow. Near-continuum flows of argon, dissociating nitrogen, and dissociating carbon dioxide over a wedge with Kn $\sim 5 \times 10^{-4}$ were examined there, providing therefore good grounds for the DSMC model validation.

The work on validation of DSMC models of real gas effects by comparisons with the experimental data of [1] was started in [2], where a nitrogen flow in a wide range of wedge angles was studied by the DSMC method. In DSMC computations, the real gas effects were described with the use of the Larsen-Borgnakke model (LB) [3] for simulation of translational-rotational and translational-vibrational energy transfer and Total Collision Energy model (TCE) [4] for modeling chemical reactions. Two types of the description of internal energy of molecules were used: continuous (classical) and discrete (quantum). Note, in the case of the continuous description, the LB and TCE models were used in the traditional form, whereas in the case of the discrete description, the models were used in a modified form, which allows one to preserve proper thermal relaxation and chemical rates in equilibrium [5]. A comparison of DSMC results with experimental data showed that the computations offer a qualitatively adequate prediction of the nonlinear dependence of the stand-off distance on the wedge angle observed in the experiments. Qualitatively, the results are different: numerical simulations predict a smaller stand-off distance of the shock wave for all wedge angles and a greater detachment angle than that observed in the experiment. An assumption was put forward in [2] that a possible reason for this difference is the fact that the DSMC models of real gas effects used ignore the effect of vibration-dissociation coupling (VDC) [6].

The present study is a continuation of [2]. The main challenge is to study the VDC effect on the shock-detachment process. For this purpose, a chemically reacting flow around a wedge is numerically studied in the present paper with

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the use of a new vibrationally-favored model of chemical reactions presented in [7] (below, it will be called the *VDC model*), and the numerical results are compared with experimental data of [1] and with DSMC results obtained with the use of the TCE model. Another possible reason of disagreement between numerical data and experimental results in [2] is the inconsistency of the chemical reaction rates used in calculations to real reaction rates. Therefore, the sensitivity of DSMC results to the choice of chemical reaction rates for the nitrogen flow was additionally considered: the flow around the wedge was simulated with an alternative set of reaction rates.

FLOW CONDITIONS AND COMPUTATIONAL METHOD

The experiments [1] were performed on a wedge of length $w = 0.051$ m. Since the aspect ratio of the wedge was $L/w = 3$ (the wedge spanwise dimension was $L = 0.152$ m), the flow in the symmetry plane could be considered as two-dimensional. A 2D statement was used, therefore, in the present study.

The free stream conditions were assumed as follows. The values of the main parameters (velocity V_∞=5500 m/s, temperature $T_\infty = 1100$ K, density ρ_∞=0.026 kg/m^3, and flow composition: 31.9 $mole/kg$ of N_2 and 7.7 $mole/kg$ of N) were taken from [1]. Based on these parameters and wedge length, the free stream Mach and Knudsen numbers are M=7.7 and Kn=6.52×10^{-4}, respectively.

The following dissociation reactions were taken into account n studying the chemically reacting nitrogen flow:

1. $N_2 + N_2 \longrightarrow N + N + N_2$
2. $N_2 + N \longrightarrow N + N + N$

The chemical reaction rate constants in all computations were taken from [8], except for the case where alternative reaction rates taken from [9] were used. The recombination reactions were not modeled in the present study. Under given conditions, recombination is essential in the boundary layer only, which was shown in [2].

The DSMC computations were performed using the SMILE software system [10] developed at Institute of Theoretical and Applied Mechanics (ITAM, Novosibirsk) and based on the majorant frequency scheme. SMILE employs two independent grids adapted in the course of computation: the first one to organize particle collisions, and the second one for sampling of macroparameters. Both grids are based on uniform rectangular background cells, which are split into smaller cells, if necessary.

The following models and features of the numerical algorithm were employed in the computations:

- Variable Hard Sphere molecular collision [4] model;
- diffuse reflection model with complete accommodation of translational and internal energies at the wedge surface;
- discrete description of rotational and vibrational energies of molecules;
- LB model for translational-rotational and translational-vibrational energy transfer with temperature-dependent rotational and vibrational collision numbers (vibrational collision numbers are corrected according to the procedure of [5]);
- two models of chemical reactions: TCE [4] and VDC [7] models with a modified form of the reaction probability according to the algorithm described in [5] in order to capture the correct equilibrium reaction rates;
- collision selection methodology of [5], which allows obtaining correct rates of multiple relaxation processes

Most of the DSMC computations were performed on a multiprocessor computer MVS1000M at the Interdepartmental Supercomputer Center (Moscow, Russia). About 20 million of simulated particles and about 5 million collisional cells were used in a typical DSMC computation. The numerical accuracy issues are discussed in detail in [2].

RESULTS

Let us first consider the general structure of the flow about a wedge. The dissociating nitrogen flow pattern obtained by DSMC computations with the TCE model for different wedge angles is demonstrated by the Mach number flowfields plotted in Fig. 1. For an angle of attack of 47°, the flow pattern with an attached wave is formed. For a wedge angle of 53.5°, one can observe the flow pattern with a slightly detached shock wave. The stand-off distance of the wave for a wedge angle of 62.5° is about 15 % of the wedge length. The main qualitative difference of the flowfields of a dissociating diatomic gas from those of a nonreacting monatomic gas is the shape of isolines immediately behind

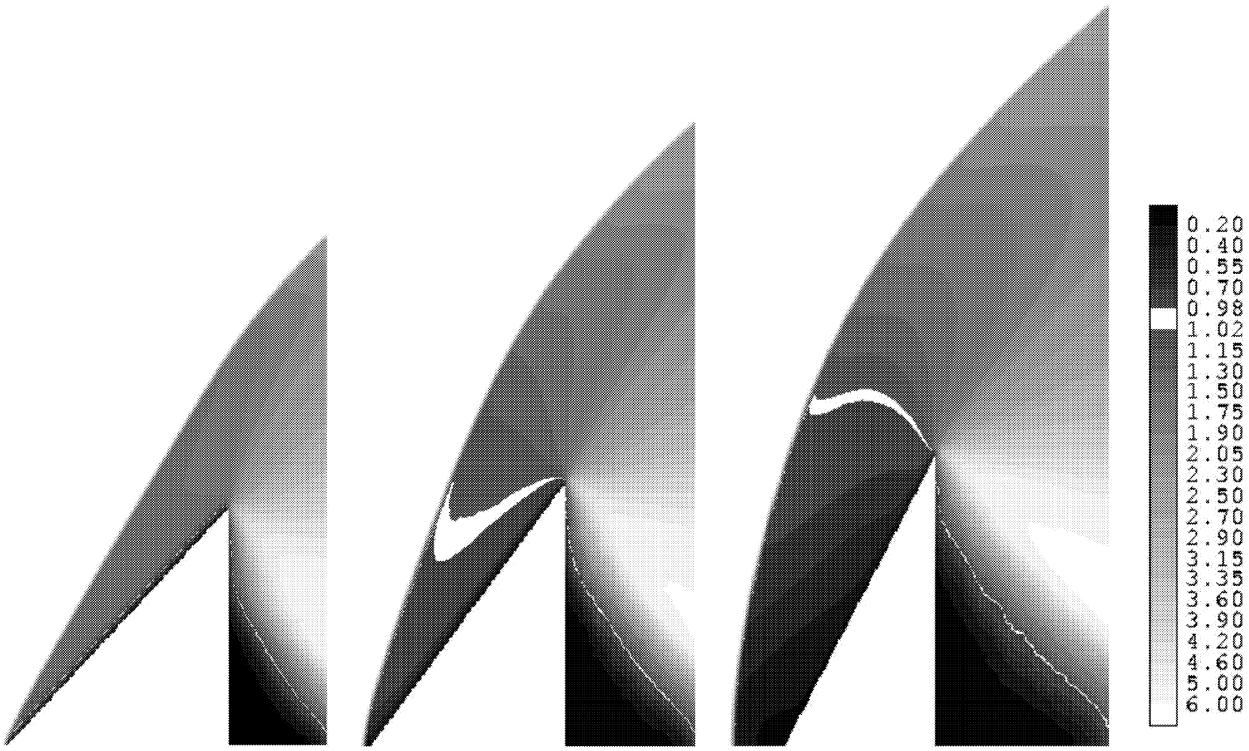

FIGURE 1. Mach number for $\delta_w = 47^\circ$ (left), 53.5° (middle), and 62.5° (right) for reacting case (TCE).

the shock-wave front (see [2]). The Mach number behind the shock-wave front in the monatomic gas decreases monotonically with increasing distance from the front (in the normal direction). In dissociating nitrogen, the Mach number behind the shock wave first slightly increases and then gradually decreases. The growth of the Mach number behind the shock-wave front is associated with relaxation processes (relaxation of internal energy and dissociative relaxation) behind the front (see [1]).

To study the effect of the chemical reaction model used in the computations of the flow, the following cases were considered:

1. nonreacting flow;
2. reacting flow (with the TCE model for chemical reactions);
3. reacting flow (with the VDC model for chemical reactions).

Note that the VDC model has a free nonnegative parameter ϕ, which determines the degree of vibrational favoring: the greater ϕ, the greater this degree. If $\phi = 0$, the model still has some degree of vibrational favoring and is not equivalent to the TCE model. The values of the VDC parameter $\phi = 0$, 1, and 3 were used in the present study (in what follows, cases with these values of the VDC parameter are denoted by VDC0, VDC1, and VDC3, respectively).

Figure 2 shows the fields of translational temperature for the flow with a strongly detached shock wave (δ_w=62.5°) for the reacting (TCE), reacting (VDC3), and nonreacting cases. Allowance for chemical reactions significantly decreases the temperature behind the shock-wave front. A more important fact for this study is that the chemical reactions lead to a significant decrease in the stand-off distance. In the VDC3 case, the shock-wave stand-off distance is greater than that predicted by the TCE model, and the temperature behind the wave front is higher. In this meaning, the VDC3 case occupies an intermediate position between the TCE case and non-reacting case.

The results obtained with the use of TCE and VDC models can be compared in more detail with the help of profiles of macroparameters along the stagnation streamline (the flow direction is from left to right; $X = 0$ is the stagnation point). The profiles of translational temperature for all cases considered and for a wedge angle of 62.5° are plotted in Fig. 3. The minimum stand-off distance is observed in computations with the TCE model (about 8 mm). In computations with the VDC model, the stand-off distance is greater; as the VDC parameter ϕ increases from 0 to 3, the

FIGURE 2. Translational temperature for $\delta_w = 62.5^\circ$: nonreacting case - left, reacting case (VDC3) - middle, reacting case (TCE) - right.

stand-off distance increases approximately from 9 mm to 11.5 mm. The stand-off distance reaches the highest value (approximately 17 mm) in the non-reacting case. In all four reacting cases (TCE and VDC), the temperature decreases behind the shock-wave front. The most intense decrease in temperature is observed in the TCE case. For the VDC model, the temperature behind the wave decreases less drastically than that in the TCE case; the higher the value of the VDC parameter, the less significant decrease in temperature behind the wave. In the non-reacting case, the temperature behind the shock-wave front reaches a constant value and decreases only in the vicinity of the stagnation point (inside the boundary layer). These results can be explained by the fact that the higher the degree of vibration-dissociation coupling in the model of chemical reactions, the slower the dissociation behind the shock-wave front, and hence, the closer the results to the non-reacting case.

This conclusion is supported by the profiles of atomic nitrogen mass fractions for all four reacting cases also shown in Fig. 3. Indeed, the atomic nitrogen mass fraction behind the shock wave reaches the maximum value equal to 0.33 if the TCE model of chemical reactions is used. With the use of the VDC model, the maximum values of the mass fraction do not exceed 0.31, 0.30, and 0.27 for ϕ =0, 1, and 3, respectively. Thus, allowance for vibration-dissociation coupling reduces the rate of dissociation behind the shock-wave front.

The experimental and numerical curves for the stand-off distance versus the wedge angle for a nitrogen flow are plotted in Fig. 4. First, note that the computations predict an almost linear dependence of the stand-off distance on the wedge angle for the nonreacting gas. Chemical reactions result in a slower and nonlinear increase in the stand-off distance with increasing wedge angle.

A comparison of numerical simulation results for the reacting TCE case with the stand-off distance measured in the experiment of [1] shows that numerical simulations offer a qualitatively correct description of the nonlinear dependence of the stand-off distance on the wedge angle, which is in agreement with the conclusions of [1]. Note, nevertheless, a significant quantitative difference between the computational results and experimental data. First, the computations predict detachment at a higher wedge angle ($\delta_w > 47^\circ$) than the experiment ($\delta_w \sim 45^\circ$). Second, the computations underpredict the stand-off distance. Almost for all values of the wedge angle, the computation results are outside the measurement error for the stand-off distance.

If the VDC model is used, the stand-off distance increases, as compared to the TCE case. The higher the VDC parameter, the greater the stand-off distance, which is illustrated by computations for wedge angles of 53.5° and 62.5°. VDC0 computations yield a result lying slightly outside the measurement-error bar for an angle of 62.5° but underpredicts the stand-off distance for an angle of 53.5° almost by a factor of 2. The results of VDC1 computations for

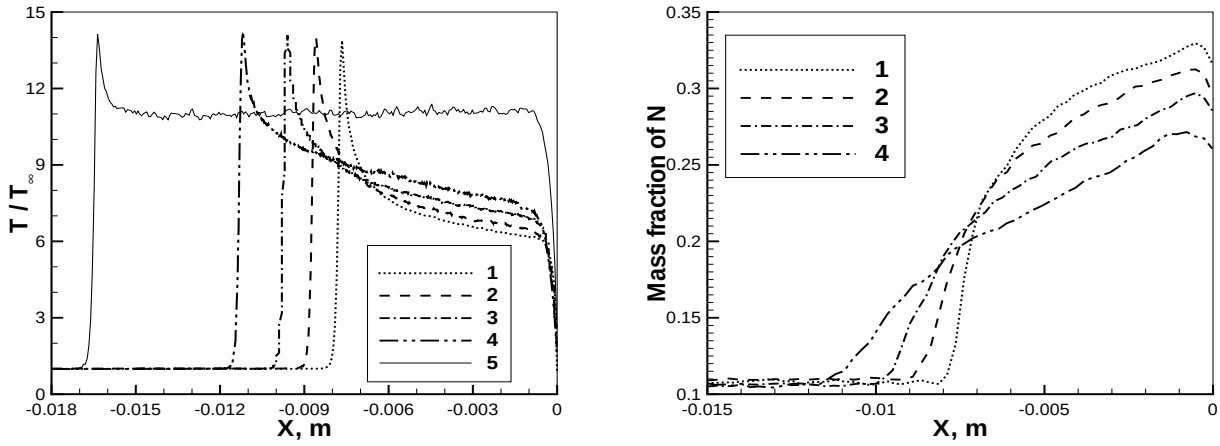

FIGURE 3. Translational temperature (left) and atomic nitrogen mass fraction (right) along the stagnation streamline, $\delta_w = 62.5^\circ$. 1 - TCE, 2 - VDC0, 3 - VDC1, 4 - VDC3, 5 - nonreacting case.

an angle of 62.5° are within the measurement error. VDC3 computations yield excellent agreement with experimental data for an angle of 53.5° but significantly (by more than 15 %) overpredicts them for a wedge angle of 62.5°. Note that the computation results for all cases for an angle of 47° predict a flow pattern with an attached shock. This means that the detachment angle for all cases considered is not smaller than 47°, which is approximately two degrees higher than in the experiment. Another significant difference of the computation results for all reacting cases from experimental data is a more rapid growth of the stand-off distance with increasing wedge angle (for $\delta_w > 53.5^\circ$).

Figure 4 shows the results of modeling with the TCE model and reaction rates of [9]. One can clearly see that the use of alternative reaction rates leads to a certain increase in the stand-off distance for angles of 53.5 and 62.5° but does not eliminate the difference between numerical results and experimental data, which were mentioned above.

Thus, we can conclude that the most probable main reason for the difference between the simulations and the experimental results of [1] is the inaccuracy in free-stream conditions reported there, which was discussed in [2]. To perform further numerical studies, the free-stream conditions of the experiment have to be refined.

CONCLUSIONS

The effect of vibration-dissociation coupling on shock detachment for a chemically reacting flow around a wedge was considered in the present paper. A steady hypersonic nitrogen 2D flow around a wedge with a Knudsen number $\mathrm{Kn} = 6.52 \times 10^{-4}$ was numerically studied by the DSMC method. Two models of chemical reactions were used in the computations: modified Total Collision Energy model [5] and and vibrationally-favored model presented in [7]. The second model has a free VDC parameter determining the degree of vibration-dissociation coupling.

The computation results showed that allowance for vibration-dissociation coupling in simulations leads to a decrease in chemical reaction rates behind the shock wave, which yields a significantly greater stand-off distance. Allowance for vibration-dissociation coupling also improves the agreement between numerical and experimental data on the stand-off distance for some values of the wedge angle. In particular, very good agreement with experimental results is observed for a wedge angle of 62.5° and VDC parameter $\phi = 1$ and for a wedge angle of 53.5° and $\phi = 3$. Nevertheless, for all fixed values of the VDC parameter, the computations yield dependences of the stand-off distance on the wedge angle, which significantly differ from the experimental curve. First, detachment in computations occurs at an angle approximately two degrees higher than that in the experiment; second, the computations predict a more rapid growth of the stand-off distance with increasing wedge angle.

The influence of the rate constant of chemical reactions on modeling results was also examined in the paper. The use of alternative reaction rates [9] in computations slightly increases the stand-off distance but does not eliminate qualitative differences from experimental data.

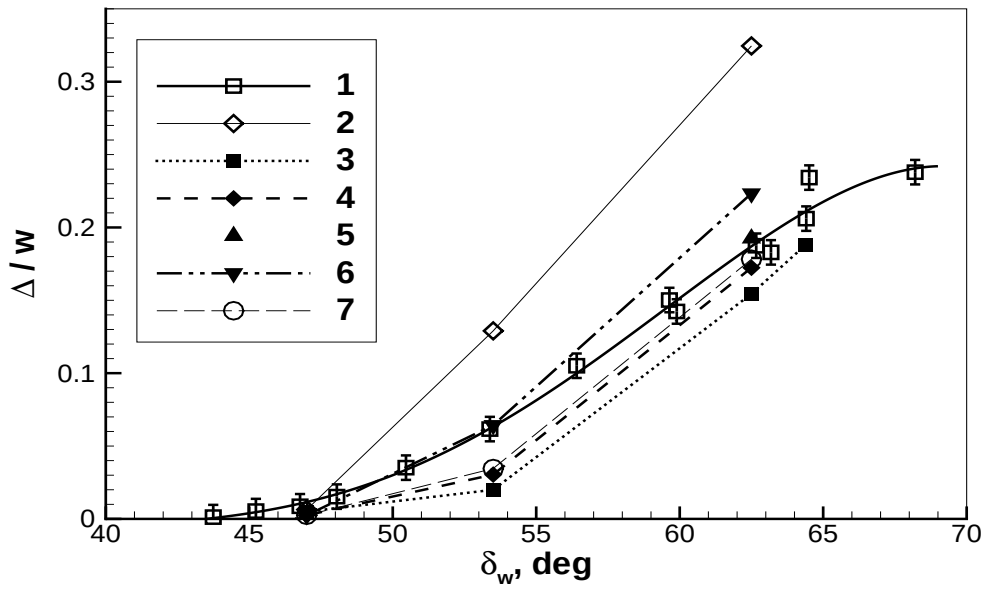

FIGURE 4. Stand-off distance. 1 - measurements of [1], 2 - nonreacting case, 3 - TCE, 4 - VDC0, 5 - VDC1, 6 - VDC3, 7 - TCE with alternative reaction rates.

Further activities on validation of the models of the DSMC method by comparisons with experimental data of Hornung and Smith require refinement of experimental free-stream conditions. For this purpose, a detailed Navier-Stokes computation of the nozzle flow with real gas effects is planned.

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